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Circulant preconditioned WR-BVM methods for ODE systems[☆]

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Abstract

We consider the solution of a system of ordinary differential equations (ODEs) by waveform relaxation (WR) iterations in conjunction with boundary value methods (BVMs). The WR method is a continuous-in-time analogue of the stationary method and it iterates with functions. In each WR iteration, we use BVMs to discretize systems of ODEs. BVMs are relatively new ODE solvers based on linear multistep formulae. In this paper, we discuss the use of the generalized minimal residual (GMRES) method with block-circulant–circulant-block preconditioners for solving the linear systems arising from the application of BVMs in each WR iteration. These preconditioners are effective in speeding up the convergence rate of the GMRES method. Numerical experiments are presented to illustrate the effectiveness of our methods.

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1. Introduction

Consider a system of linear differential equations

$$\begin{cases} \frac{dy(t)}{dt} + Qy(t) = g(t), & t \in (t_0, T], \\ y(t_0) = z, \end{cases} \quad (1)$$

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where $\mathbf{y}(t), \mathbf{g}(t) : \mathbb{R} \rightarrow \mathbb{R}^m$, $\mathbf{z} \in \mathbb{R}^m$, and $Q \in \mathbb{R}^{m \times m}$. Splitting the matrix Q as

$$Q = M - N \quad (2)$$

and reconstructing (1) by a method of successive approximations, we have

$$\begin{cases} \frac{d\mathbf{y}^{(k+1)}(t)}{dt} + M\mathbf{y}^{(k+1)}(t) = N\mathbf{y}^{(k)}(t) + \mathbf{g}(t), & t \in (t_0, T], \\ \mathbf{y}^{(k+1)}(t_0) = \mathbf{z}, \end{cases} \quad (3)$$

where $k = 0, 1, \dots$, and $\mathbf{y}^{(0)}$ is an initial guess, usually given by $\mathbf{y}^{(0)}(t) \equiv \mathbf{z}$ for $t \in [t_0, T]$. The approximation (3) is called the *waveform relaxation* (WR) method. This technique was originated from electrical network simulation, see [9]. It is a continuous-in-time analogue of the stationary method and it iterates with functions.

WR methods can be very effective if they converge fast. Unfortunately, this is not always the case. The convergence behavior of WR methods has been studied extensively in many papers [10–12]. To accelerate the convergence, Vandewalle in [14] used the multigrid techniques in the context of WR methods for parabolic partial differential equations. The effectiveness of preconditioning WR methods for solving (1) was discussed in [3].

The Jacobi and Gauss–Seidel versions of the WR technique are classical methods. To be precise, the matrix Q is decomposed as $Q = L + D + U$, where D is a diagonal matrix, L is a strictly lower triangular matrix and U is a strictly upper triangular matrix. The splittings

$$M = D, \quad N = -L - U$$

and

$$M = L + D, \quad N = -U$$

define, respectively, the Jacobi and Gauss–Seidel WR iterations.

In this paper, we use a circulant splitting of Q to construct a new scheme of the WR method. More precisely, in (2), we use T. Chan's circulant approximation for Q as our splitting matrix M , i.e., $M \equiv c(Q)$, where $c(Q)$ is the minimizer of

$$\|Q - C\|_F$$

over all circulant matrices $C \in \mathbb{R}^{m \times m}$ under the Frobenius norm $\|\cdot\|_F$, see [5,7]. We remark that if $Q = [q_{j,k}]_{j,k=1}^m$, the diagonals of $c(Q)$ are given by

$$c_i = \frac{1}{m} \sum_{j-k \equiv i \pmod{m}} q_{j,k}, \quad i = 0, \dots, m-1.$$

The reason that we use T. Chan's circulant approximation $c(Q)$ is because it is well defined for any matrix Q and moreover, it can easily give us an error estimate of WR iterations, see Section 2.

Let $M \equiv c(Q)$ and $N \equiv c(Q) - Q$, the splitting in (2) becomes

$$Q = c(Q) - (c(Q) - Q).$$

After the splitting, the *boundary value method* (BVM), see [2,8], is applied to each WR iteration (3). The BVM requires the solution of nonsymmetric linear systems that are often large and sparse. We use the generalized minimal residual (GMRES) method with block-circulant–circulant-block preconditioners to solve these linear systems.

The paper is organized as follows. In Section 2, we give an error estimate of the WR iterations. In Section 3, we introduce the BVM and the Strang-type circulant preconditioner. The invertibility of the Strang-type preconditioner is discussed in Section 4. The convergence rate and operation cost of the preconditioned GMRES method are studied in Section 5. Finally, numerical experiments are given in Section 6 to illustrate the effectiveness of our methods.

2. Error estimate of WR iterations

We shall consider the space of continuous functions $\mathcal{C}[t_0, T]$ equipped with the sup-norm

$$\|\mathbf{y}(t)\|_T \equiv \sup\{\|\mathbf{y}(t)\| : t \in [t_0, T]\},$$

where $\mathbf{y}(t) : \mathbb{R} \rightarrow \mathbb{R}^m$ and $\|\cdot\|$ is some norm on \mathbb{R}^m . We will use the norm $\|\cdot\|_2$ in the following discussion. It is well known [11] that if the iterations defined by (3) converge, the error of the k th WR iteration $\mathbf{y}^{(k)}(t)$ can be bounded by

$$\|\mathbf{y}(t) - \mathbf{y}^{(k)}(t)\|_T \leq \frac{(C(T - t_0))^k}{k!} \|\mathbf{y}(t) - \mathbf{y}^{(0)}(t)\|_T,$$

where $\mathbf{y}(t)$ is the solution of (1) and C is a constant such that

$$\|e^{-Mt}N\|_T \leq C.$$

Here $\|\cdot\|_T$ is the corresponding induced matrix norm. Note that if C is large, then finding \mathbf{y} through the WR iterations can be ill-conditioned and correspondingly the actual algorithm (based on numerical integration) will be numerically unstable. Usually, it is not easy to estimate C , see [3,11].

In the following, we give a computable bound on $\|e^{-Mt}N\|_T$ for our method. It is well-known that any $m \times m$ circulant matrix can be diagonalized by the $m \times m$ Fourier matrix F_m (see [5,7]).

Hence, we have the following decomposition

$$M \equiv c(Q) = F_m A_M F_m^*, \quad (4)$$

where $A_M = \text{diag}(\lambda_1, \lambda_2, \dots, \lambda_m)$ is a diagonal matrix holding the eigenvalues of M . By using (4), we obtain

$$\begin{aligned} \|e^{-Mt}N\|_T &= \sup_{\|\mathbf{y}(t)\|_2=1} \sup_{t \in [t_0, T]} \|e^{-Mt}N\mathbf{y}(t)\|_2 \\ &\leq \sup_{t \in [t_0, T]} \|e^{-F_m A_M F_m^* t}N\|_2 \\ &= \sup_{t \in [t_0, T]} \|F_m e^{-A_M t} F_m^* N\|_2 \end{aligned}$$

$$\begin{aligned}
&\leq \sup_{t \in [t_0, T]} \{ \|\text{diag}(e^{-\lambda_1(M)t}, \dots, e^{-\lambda_m(M)t})\|_2 \cdot \|N\|_2 \} \\
&= \sup_{t \in [t_0, T]} \sqrt{\max_{1 \leq i \leq m} e^{-2\Re(\lambda_i(M))t}} \cdot \|N\|_2 \\
&\leq \|N\|_F = \|Q - c(Q)\|_F.
\end{aligned}$$

where $\Re(\cdot)$ is the real part of a complex number. Thus the approximation $\|Q - c(Q)\|_F$ gives a bound on the accuracy of the WR method.

3. BVM and circulant preconditioner

In WR iterations, BVMs are proposed to solve a series of ODE systems (3). The BVMs are numerical methods based on linear multistep formulae (LMF) for solving ODEs. A BVM approximates the solution of (3) by means of a discrete boundary value problem. By using a v -step LMF over a uniform mesh

$$t_j = t_0 + jh, \quad j = 0, \dots, s,$$

where $h = (T - t_0)/s$ is the stepsize, we have

$$\sum_{i=-v}^{\mu-v} \alpha_{i+v} \mathbf{y}_{n+i}^{(k+1)} = h \sum_{i=-v}^{\mu-v} \beta_{i+v} \mathbf{f}_{n+i}, \quad n = v, \dots, s - \mu + v \quad (5)$$

with boundary values

$$\mathbf{y}_0^{(k+1)}, \dots, \mathbf{y}_{v-1}^{(k+1)}, \quad \mathbf{y}_{s-\mu+v+1}^{(k+1)}, \dots, \mathbf{y}_s^{(k+1)}. \quad (6)$$

In (5), $\mathbf{y}_n^{(k+1)}$ is an approximation to the true solution $\mathbf{y}^{(k+1)}(t_n)$ of (3) and

$$\mathbf{f}_n \equiv -M\mathbf{y}_n^{(k+1)} + \mathbf{u}_n^{(k)},$$

where

$$\mathbf{u}_n^{(k)} \equiv N\mathbf{y}_n^{(k)} + \mathbf{g}(t_n)$$

and $\mathbf{y}_n^{(k)} \approx \mathbf{y}^{(k)}(t_n)$ can be obtained from the k th WR iteration.

For the boundary values (6), the iteration (3) only provides one initial condition

$$\mathbf{y}_0^{(k+1)} \equiv \mathbf{y}^{(k+1)}(t_0) = \mathbf{z}. \quad (7)$$

To obtain the other boundary values, we add two sets of initial and final additional difference equations with the same order of accuracy of (5), see [2]. Let them be denoted by

$$\sum_{i=0}^{\mu} \alpha_i^{(j)} \mathbf{y}_i^{(k+1)} = h \sum_{i=0}^{\mu} \beta_i^{(j)} \mathbf{f}_i, \quad j = 1, \dots, v-1 \quad (8)$$

and

$$\sum_{i=0}^{\mu} \alpha_{\mu-i}^{(j)} \mathbf{y}_{s-i}^{(k+1)} = h \sum_{i=0}^{\mu} \beta_{\mu-i}^{(j)} \mathbf{f}_{s-i}, \quad j = s - \mu + v + 1, \dots, s. \quad (9)$$

By combining (5), (7)–(9), we obtain the following linear system:

$$T\mathbf{y}^{(k+1)} = G\mathbf{y}^{(k)} + \mathbf{d}, \quad (10)$$

where

$$T = A \otimes I_m + hB \otimes M \quad (11)$$

with the identity matrix $I_m \in \mathbb{R}^{m \times m}$,

$$\mathbf{y}^{(k+1)} = ((\mathbf{y}_0^{(k+1)})^T, \dots, (\mathbf{y}_s^{(k+1)})^T)^T \in \mathbb{R}^{(s+1)m},$$

$$G = -h(B \otimes N),$$

$$\mathbf{d} = \mathbf{e}_1 \otimes \mathbf{z} + h(B \otimes I_m)\mathbf{g} \in \mathbb{R}^{(s+1)m}$$

with $\mathbf{e}_1 = (1, 0, \dots, 0)^T \in \mathbb{R}^{(s+1)}$ and $\mathbf{g} = (\mathbf{g}(t_0), \mathbf{g}(t_1), \dots, \mathbf{g}(t_s))^T \in \mathbb{R}^{(s+1)m}$.

In (11), the matrix $A \in \mathbb{R}^{(s+1) \times (s+1)}$ is defined by

$$A \equiv \begin{bmatrix} 1 & \cdots & 0 & & & \\ \alpha_0^{(1)} & \cdots & \alpha_\mu^{(1)} & & & \\ \vdots & \vdots & \vdots & & & \\ \alpha_0^{(v-1)} & \cdots & \alpha_\mu^{(v-1)} & & 0 & \\ \alpha_0 & \cdots & \alpha_\mu & & & \\ & \alpha_0 & \cdots & \alpha_\mu & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & \ddots \\ & & & & \alpha_0 & \cdots & \alpha_\mu \\ & & 0 & \alpha_0^{(s-\mu+v+1)} & \cdots & \alpha_\mu^{(s-\mu+v+1)} \\ & & & \vdots & \vdots & \vdots \\ & & & \alpha_0^{(s)} & \cdots & \alpha_\mu^{(s)} \end{bmatrix}$$

and $B \in \mathbb{R}^{(s+1) \times (s+1)}$ is defined similarly by replacing $\{\alpha_i\}_{i=0}^\mu$ in A by $\{\beta_i\}_{i=0}^\mu$ and setting all elements of the first row of B to zero. Note that A and B are Toeplitz-like matrices. We remark that a matrix is said to be Toeplitz if its entries are constant along its diagonals and a matrix is said to be Toeplitz-like

if it is a Toeplitz matrix with small perturbations. Obviously, (10) is a classical stationary iteration for linear systems. It is well known that the convergence of such an iteration requires $\rho(T^{-1}G) < 1$, where $\rho(\cdot)$ is the spectral radius. Since the size of the matrix T is very large when h is small and (or) m is large, the cost of using a direct method to solve the system (10) can be very high, see numerical comparisons in [1,6]. Therefore, Krylov subspace methods, such as the GMRES method in [13], were proposed to solve (10). In order to speed up the convergence rate of Krylov subspace methods, we use the Strang-type block-circulant preconditioner. We note that for the splitting

$$Q = c(Q) - (c(Q) - Q),$$

the iteration matrix in (11) becomes

$$T = A \otimes I_m + hB \otimes c(Q) \quad (12)$$

which is a block-Toeplitz–Toeplitz-block matrix with small perturbations. To solve the linear system (10) with T given by (12), we propose the Strang-type block-circulant preconditioner S as follows:

$$S = s(A) \otimes I_m + hs(B) \otimes c(Q), \quad (13)$$

where

$$s(A) \equiv \begin{bmatrix} \alpha_v & \cdots & \alpha_\mu & & \alpha_0 & \cdots & \alpha_{v-1} \\ \vdots & \ddots & & \ddots & & \ddots & \vdots \\ \alpha_0 & & \ddots & & \ddots & & \alpha_0 \\ & \ddots & & \ddots & & \ddots & 0 \\ & & \ddots & & \ddots & \ddots & \\ & 0 & & \ddots & & \ddots & \\ \alpha_\mu & & & \ddots & & \ddots & \alpha_\mu \\ \vdots & \ddots & & & \ddots & \ddots & \vdots \\ \alpha_{v+1} & \cdots & \alpha_\mu & & \alpha_0 & \cdots & \alpha_v \end{bmatrix}$$

with $\{\alpha_i\}_{i=0}^\mu$ being the coefficients given in (5), and $s(B)$ has the same structure as $s(A)$ except that $\{\alpha_i\}_{i=0}^\mu$ are replaced by $\{\beta_i\}_{i=0}^\mu$. We remark that S is already a block-circulant–circulant-block matrix which can be diagonalized by the Fourier matrix, see [4,5,7] and Section 5.

4. Invertibility of preconditioner S

It can be proved that under stability assumption on a given BVM, the Strang-type preconditioner is invertible. The stability of a BVM is closely related to two characteristic polynomials $\rho(z)$ and

$\sigma(z)$ defined by

$$\rho(z) \equiv z^v \sum_{i=-v}^{\mu-v} \alpha_{i+v} z^i \quad \text{and} \quad \sigma(z) \equiv z^v \sum_{i=-v}^{\mu-v} \beta_{i+v} z^i, \quad (14)$$

where $\{\alpha_i\}_{i=0}^{\mu}$ and $\{\beta_i\}_{i=0}^{\mu}$ are given in (5). The $A_{v,\mu-v}$ -stability polynomial is defined by

$$\pi(z, q) \equiv \rho(z) - q\sigma(z),$$

where $z, q \in \mathbb{C}$. Let

$$\mathbb{C}^- \equiv \{q \in \mathbb{C} : \Re(q) < 0\} \quad \text{and} \quad \mathbb{C}^+ \equiv \{q \in \mathbb{C} : \Re(q) > 0\}.$$

We have

Definition 1. Consider a BVM with characteristic polynomials $\rho(z)$ and $\sigma(z)$ defined as in (14). The region

$$\mathcal{D}_{v,\mu-v} \equiv \{q \in \mathbb{C} : \pi(z, q) \text{ has } v \text{ zeros inside } |z| = 1 \text{ and } \mu - v \text{ zeros outside } |z| = 1\}$$

is called the region of $A_{v,\mu-v}$ stability of the given BVM. Moreover, the BVM is said to be $A_{v,\mu-v}$ -stable if $\mathbb{C}^- \subseteq \mathcal{D}_{v,\mu-v}$.

Theorem 1. If the BVM for (10) is $A_{v,\mu-v}$ -stable and all eigenvalues of $M \equiv c(Q)$ satisfy

$$\lambda_k(M) \in \mathbb{C}^+, \quad (15)$$

for $k = 1, \dots, m$, then the preconditioner S defined by (13) is invertible.

Proof. Follows directly from the proof of Theorem 1 in [6]. \square

Since $c(Q)$ is a circulant matrix, it can be diagonalized by the Fourier matrix F_m [5]. We have

$$M \equiv c(Q) = F_m A_m F_m^*,$$

where

$$A_M = \text{diag}(\lambda_1(M), \lambda_2(M), \dots, \lambda_m(M))$$

is a diagonal matrix holding the eigenvalues of M . We note that A_M can be obtained by applying one fast Fourier transform (FFT) of length m on the first column of M , see [5,7]. Thus it is easy to check whether (15) is satisfied. In case it is not, i.e., there exist $\lambda_l(M)$ such that $\lambda_l(M) \notin \mathbb{C}^+$, then we can “move” them into \mathbb{C}^+ by subtracting $\lambda_{\min} - \varepsilon$ from the main diagonal of the matrix M , where

$$\lambda_{\min} = \min_l \{\Re(\lambda_l(M)) : \lambda_l(M) \notin \mathbb{C}^+\}$$

and ε is a positive real number. Obviously, all the eigenvalues of the matrix

$$\tilde{M} \equiv M - (\lambda_{\min} - \varepsilon)I_m \quad (16)$$

are in \mathbb{C}^+ . Hence, Theorem 1 can still be applied to the new splitting

$$Q = \tilde{M} - \tilde{N},$$

where \tilde{M} is given by (16) and $\tilde{N} = N - (\lambda_{\min} - \varepsilon)I_m$.

5. Convergence rate and operation cost

The convergence rate of the GMRES method depends on the spectrum of the preconditioned matrix $S^{-1}T$ where T is defined by (12) and S is defined by (13). We have the following theorem.

Theorem 2. *The preconditioned matrix $S^{-1}T$ can be decomposed as $S^{-1}T = I + L$, where I is the identity matrix and $\text{rank}(L) \leq 2m\mu$. If the GMRES method is applied to solving*

$$S^{-1}T\bar{\mathbf{y}}^{(k+1)} = S^{-1}\bar{\mathbf{b}},$$

the method will converge in at most $2m\mu + 1$ iterations in exact arithmetic.

Proof. Follows directly from the proof of Theorem 2 in [6]. \square

We should emphasize that the numerical tests in Section 6 show a much faster convergence rate than that predicted by the estimate provided by Theorem 2.

Now, we study the operation cost in each iteration of the GMRES method. Since $s(A)$ and $s(B)$ are both circulant matrices, we have the following decompositions:

$$s(A) = F_{s+1}A_AF_{s+1}^*, \quad s(B) = F_{s+1}A_BF_{s+1}^*, \quad (17)$$

where A_A and A_B are diagonal matrices containing the eigenvalues of $s(A)$ and $s(B)$, respectively, and F_{s+1} is the $(s+1)$ -by- $(s+1)$ Fourier matrix. The matrix-vector multiplication $S^{-1}(T\mathbf{v})$ for some vector \mathbf{v} is the main work in each iteration of the GMRES method (see [5,7], for examples). Since the matrix $M \equiv c(Q)$ is a circulant matrix, by using (4) and (17), we have

$$S^{-1}(T\mathbf{v}) = (F_{s+1} \otimes F_m)(A_A \otimes I_m + hA_B \otimes A_M)^{-1}(F_{s+1}^* \otimes F_m^*)(T\mathbf{v}).$$

By using the FFT, S^{-1} can be calculated in $\mathcal{O}(ms \log ms)$ operations. The $T\mathbf{v}$ can also be computed in $\mathcal{O}(ms \log ms)$ operations by using Strang's embedding algorithm with FFTs, see [4,5,7]. Therefore, it requires $\mathcal{O}(ms \log ms)$ operations to compute $S^{-1}(T\mathbf{v})$ in each iteration of the GMRES method.

6. Numerical tests

In this section, we illustrate the efficiency of our method by comparing with other classic WR iterations such as the Jacobi and Gauss–Seidel splittings. For a fair comparison, the BVM and the GMRES method with the preconditioner S are also applied to these classic WR iterations.

The BVM we used here is the fifth-order GAM which has $\mu=4$ and $\nu=2$, see [2]. All experiments are performed in MATLAB. We use the MATLAB-provided M-file “gmres” (see MATLAB on-line documentation) to solve the preconditioned systems. In our calculations, the stopping criterion in the GMRES method is

$$\frac{\|\mathbf{r}_q\|_2}{\|\mathbf{r}_0\|_2} < 10^{-6},$$

Table 1
Number of WR iterations for convergence in the given example

m	s	$M \equiv c(Q),$ $N \equiv c(Q) - Q$	Jacobi	Gauss–Seidel
20	16	4	5	4
	32	4	5	4
	64	4	5	4
	128	4	5	4
40	16	4	4	4
	32	4	4	4
	64	4	4	4
	128	4	4	4
60	16	4	4	4
	32	4	4	4
	64	4	4	4
	128	4	4	4

where \mathbf{r}_q is the residual after the q th GMRES iteration which is applied within each WR iteration, and the zero vector is the initial guess. The stopping criterion of the WR iterations is

$$\frac{\|\mathbf{y}^{(k+1)} - \mathbf{y}^{(k)}\|_2}{\|\mathbf{y}^{(k)}\|_2} \leq 10^{-6},$$

where $\mathbf{y}^{(k)}$ is the solution at the k th WR iteration.

Example. Consider

$$\begin{cases} \mathbf{y}'(t) + Q\mathbf{y}(t) = 0, & t \in (0, 1], \\ \mathbf{y}(0) = (1, 2, \dots, m)^T, \end{cases}$$

where

$$Q = \begin{bmatrix} m & \frac{-1}{1^2+2^2} & \frac{-1}{1^2+3^2} & \cdots & \frac{-1}{1^2+(m-1)^2} & \frac{-1}{1^2+m^2} \\ \frac{-1}{2^2+1^2} & m & \frac{-1}{2^2+3^2} & \frac{-1}{2^2+4^2} & \ddots & \vdots \\ \frac{-1}{3^2+1^2} & \frac{-1}{3^2+2^2} & m & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ \frac{-1}{(m-1)^2+1^2} & \ddots & \ddots & \ddots & \ddots & \frac{-1}{(m-1)^2+m^2} \\ \frac{-1}{m^2+1^2} & \cdots & \cdots & \frac{-1}{m^2+(m-2)^2} & \frac{-1}{m^2+(m-1)^2} & m \end{bmatrix}.$$

Tables 1 and 2 list, respectively, the number of WR iterations and the number of megaflops (Mflops) required for convergence with different combinations of matrix sizes m and s . As expected,

Table 2
Number of Mflops for convergence in the given example

m	s	$M \equiv c(Q),$ $N \equiv c(Q) - Q$	Jacobi	Gauss–Seidel
20	16	4.6895	5.6854	5.3076
	32	9.9054	11.354	10.552
	64	19.540	23.983	20.923
	128	38.368	44.862	44.194
40	16	9.9451	9.9335	11.319
	32	22.282	20.830	23.741
	64	40.683	43.717	46.768
	128	85.421	91.802	95.219
60	16	16.471	16.453	17.604
	32	29.654	32.014	34.385
	64	61.929	66.799	66.869
	128	129.45	139.66	139.45

Table 3
WR error estimate C in the given example

m	C
20	2.5835×10^{-1}
40	2.8808×10^{-1}
60	2.9934×10^{-1}

the number of WR iterations required for convergence remains almost constant for increasing m and s . The constant C given in Section 2 for error estimate analysis of the WR iteration is also shown in Table 3. The constant C remains roughly unchanged for different m , which is consistent with the results in Table 1. Thus, from a viewpoint of WR iterations, our new scheme is comparable with some classical schemes. However, we can easily estimate the error of our WR scheme in advance. We should emphasize that our circulant preconditioner can only speed up the convergence rate of the GMRES method no matter which kind of WR scheme is used.

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